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=> d his

     (FILE 'HOME' ENTERED AT 12:46:36 ON 01 MAY 2002)

     FILE 'REGISTRY' ENTERED AT 12:47:08 ON 01 MAY 2002
L1              STRUCTURE UPLOADED
L2            1 S L1
L3           22 S L1 FUL

     FILE 'REGISTRY' ENTERED AT 12:48:04 ON 01 MAY 2002
L4            1 S L3

     FILE 'CAPLUS' ENTERED AT 12:48:15 ON 01 MAY 2002
L5            1 S L3

     FILE 'REGISTRY' ENTERED AT 12:50:01 ON 01 MAY 2002

     FILE 'REGISTRY' ENTERED AT 12:50:58 ON 01 MAY 2002
L6              STRUCTURE UPLOADED
L7           19 S L6 FUL

     FILE 'CAPLUS' ENTERED AT 12:51:22 ON 01 MAY 2002
L8            2 S L7

=> d l6
L6 HAS NO ANSWERS
L6              STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.


=> d bib abs hitstr 1-2

L8   ANSWER 1 OF 2  CAPLUS  COPYRIGHT 2002 ACS
AN   2001:662560  CAPLUS
DN   135:352345
TI   Statistical Molecular Design, Parallel Synthesis, and Biological
     Evaluation of a Library of Thrombin Inhibitors
AU   Linusson, Anna; Gottfries, Johan; Olsson, Thomas; Oernskov, Eivor;
     Folestad, Staffan; Norden, Bo; Wold, Svante
CS   AstraZeneca R&D Molndal, Moelndal, S-431 83, Swed.
SO   Journal of Medicinal Chemistry (2001), 44(21), 3424-3439
     CODEN: JMCMAR; ISSN: 0022-2623
PB   American Chemical Society
DT   Journal
LA   English
AB   A library of thrombin inhibitors has been designed using statistical mol.
     design.  An arom. scaffold was used, with three varied positions
     corresponding to three pockets at the active site of thrombin (the S-, P-,
     and D-pockets).  The selection was performed in the building block space,
     and previously acquired data were included in the design procedure.  The
     design resulted in six, four, and six building blocks for the first (S),
     second (P), and third (D) pockets, resp.  A second round of selection
     applied to the combined selected building blocks resulted in a subset of
     18 compds.  The selected library was synthesized in parallel and biol.
     evaluated.  The compds. were analyzed with respect to their inhibition
     (pIC50) of thrombin; membrane permeability, estd. by migration behavior in
     micellar media (CE log k') and pKa; and specificity with respect to
     inhibition (Ki) of trypsin.  Multivariate QSAR studies of the responses
     yielded valuable results and information that could only be found using
     statistical mol. design in combination with multivariate anal.
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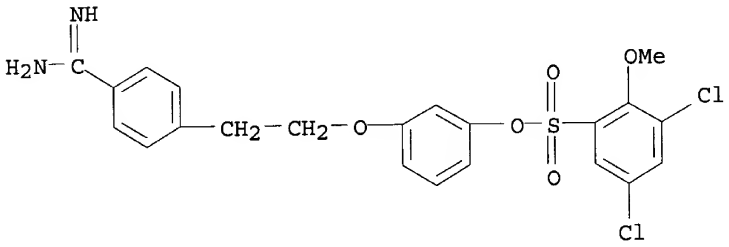
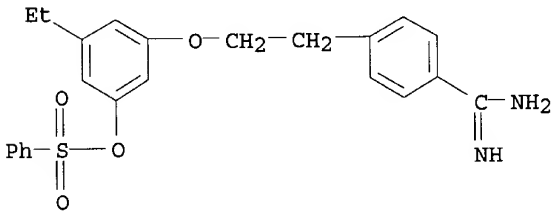
IT **372523-37-0P 372523-38-1P 372523-39-2P**
372523-40-5P 372523-41-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(statistical mol. design, parallel synthesis, and biol. evaluation of a library of thrombin inhibitors)

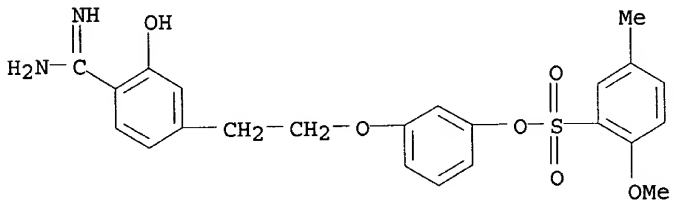
RN 372523-37-0 CAPLUS
CN Benzenesulfonic acid, 3,5-dichloro-2-methoxy-, 3-[2-[4-(aminoiminomethyl)phenyl]ethoxy]phenyl ester (9CI) (CA INDEX NAME)



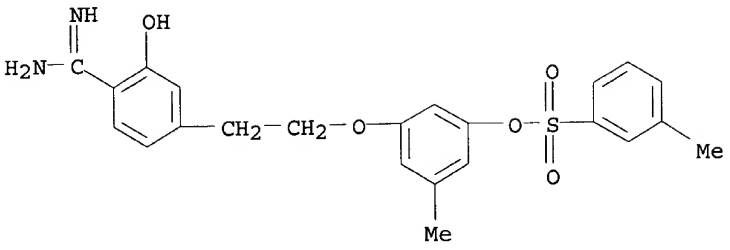
RN 372523-38-1 CAPLUS
CN Benzenecarboximidamide, 4-[2-[3-ethyl-5-[(phenylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME)



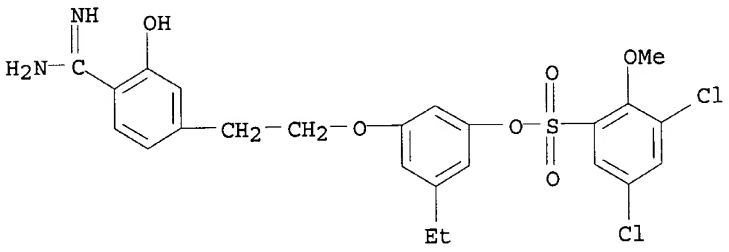
RN 372523-39-2 CAPLUS
CN Benzenesulfonic acid, 2-methoxy-5-methyl-, 3-[2-[4-(aminoiminomethyl)-3-hydroxyphenyl]ethoxy]phenyl ester (9CI) (CA INDEX NAME)



RN 372523-40-5 CAPLUS
CN Benzenesulfonic acid, 3-methyl-, 3-[2-[4-(aminoiminomethyl)-3-hydroxyphenyl]ethoxy]-5-methylphenyl ester (9CI) (CA INDEX NAME)



RN 372523-41-6 CAPLUS
CN Benzenesulfonic acid, 3,5-dichloro-2-methoxy-, 3-[2-[4-(aminoiminomethyl)-3-hydroxyphenyl]ethoxy]-5-ethylphenyl ester (9CI) (CA INDEX NAME)



RE.CNT 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2002 ACS
AN 1998:65889 CAPLUS
DN 128:127826
TI Preparation of new amidino derivatives as thrombin inhibitors
IN Antonsson, Thomas
PA Astra Aktiebolag, Swed.; Antonsson, Thomas
SO PCT Int. Appl., 108 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9801422	A1	19980115	WO 1997-SE1150	19970626
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	RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	CA 2260190	AA	19980115	CA 1997-2260190	19970626
	AU 9735628	A1	19980202	AU 1997-35628	19970626
	AU 726236	B2	20001102		
	EP 917528	A1	19990526	EP 1997-932085	19970626
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	BR 9710142	A	19990810	BR 1997-10142	19970626
	CN 1228765	A	19990915	CN 1997-197578	19970626

	JP 2000515505	T2	20001121	JP 1998-505123	19970626
	US 6221898	B1	20010424	US 1997-894833	19970829
	NO 9806180	A	19990304	NO 1998-6180	19981229
	KR 2000022437	A	20000425	KR 1998-710870	19981230
	US 2002040043	A1	20020404	US 2001-839609	20010423
PRAI	SE 1996-2646	A	19960704		
	WO 1997-SE1150	W	19970626		
	US 1997-894833	A3	19970829		

OS MARPAT 128:127826

GI

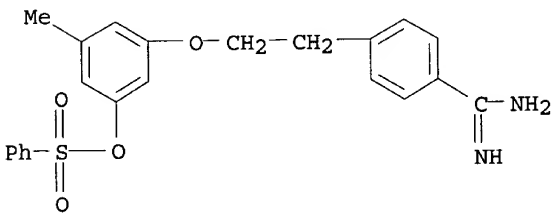
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. [I; one of R1 and R2 = Z-SO2-Ar1 and the other = R4; Z = O, NR5; R3 = Oh, halo, Cn, etc.; R4 = H, OH, halo, etc.; Ar1 = Ph, C1-3 alkylphenyl, naphthyl, etc.; R5 = H, C1-6 alkyl, Ph, C1-3 alkylphenyl; Y = O, S, S(O), SS(O)2, NR22; R22 = H, C1-4 alkyl; n = 0-4; B = II, III, IV, V; X1, X2 = a single bond, CH2], useful as competitive inhibitors of trypsin-like proteases, such as thrombin, and in particular in the treatment of conditions where inhibition of thrombin is required (e.g. thrombosis) or as anticoagulants, were prepd. Thus, reaction of 3-[2-(4-cyanophenyl)ethoxy]aniline with benzenesulfonyl chloride followed by treatment of the resulting N-{3-[2-(4-cyanophenyl)ethoxy]phenyl}benzene sulfonamide with HCl(g) in EtOH, and treating N-{3-[2-(4-ethoxyiminomethylphenyl)ethoxy]phenyl}benzenesulfonamide.HCl with NH3(g) afforded the title compd. VI. The title compds. I described herein were tested for thrombin inhibition and were found to exhibit an IC50 and/or Ki (as appropriate) of < 0.3 .mu.M.

IT **201933-66-6P 201934-29-4P 201934-30-7P**
201934-31-8P 201934-32-9P 201934-33-0P
201934-34-1P 201934-35-2P 201934-36-3P
201934-37-4P 201934-77-2P 201935-45-7P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of new amidino derivs. as thrombin inhibitors)

RN 201933-66-6 CAPLUS

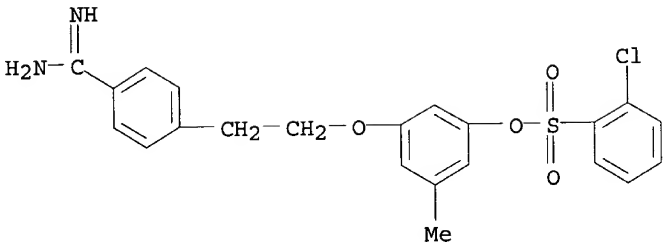
CN Benzenecarboximidamide, 4-[2-[3-methyl-5-[(phenylsulfonyl)oxy]phenoxy]ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 201934-29-4 CAPLUS

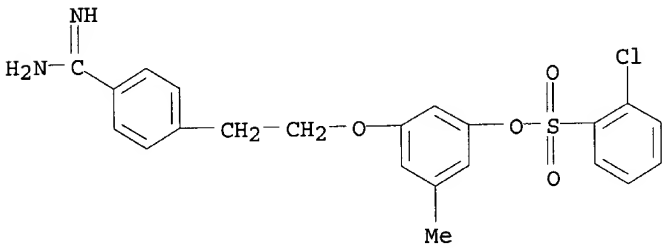
CN Benzenesulfonic acid, 2-chloro-, 3-[2-[4-(aminoiminomethyl)phenyl]ethoxy]-5-methylphenyl ester (9CI) (CA INDEX NAME)



RN 201934-30-7 CAPLUS
CN Benzenesulfonic acid, 2-chloro-, 3-[2-[4-(aminoiminomethyl)phenyl]ethoxy]-5-methylphenyl ester, monoacetate (9CI) (CA INDEX NAME)

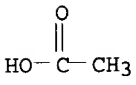
CM 1

CRN 201934-29-4
CMF C22 H21 Cl N2 O4 S

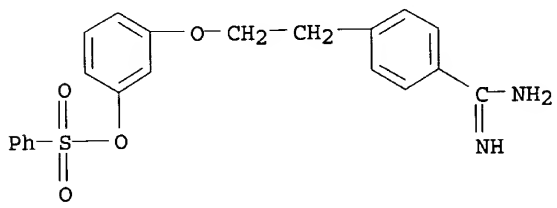


CM 2

CRN 64-19-7
CMF C2 H4 O2



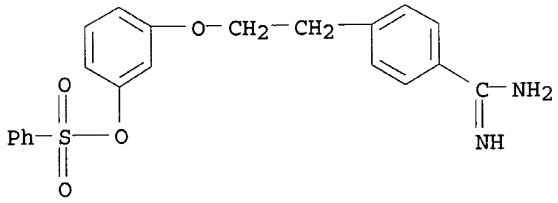
RN 201934-31-8 CAPLUS
CN Benzenecarboximidamide, 4-[2-[3-[(phenylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME)



RN 201934-32-9 CAPLUS
CN Benzenecarboximidamide, 4-[2-[3-[(phenylsulfonyl)oxy]phenoxy]ethyl]-, monoacetate (9CI) (CA INDEX NAME)

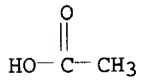
CM 1

CRN 201934-31-8
CMF C21 H20 N2 O4 S

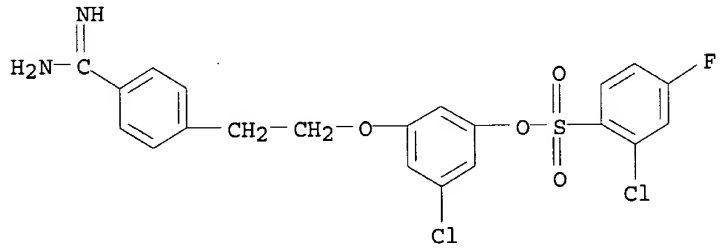


CM 2

CRN 64-19-7
CMF C2 H4 O2



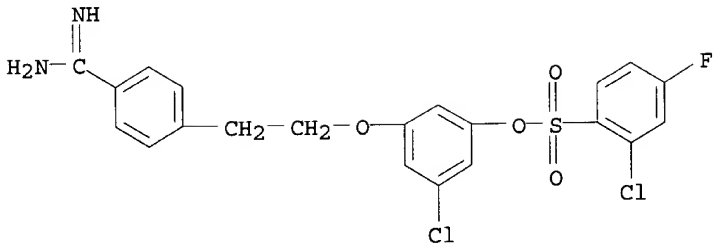
RN 201934-33-0 CAPLUS
CN Benzenesulfonic acid, 2-chloro-4-fluoro-, 3-[2-[4-(aminoiminomethyl)phenyl]ethoxy]-5-chlorophenyl ester (9CI) (CA INDEX NAME)



RN 201934-34-1 CAPLUS
CN Benzenesulfonic acid, 2-chloro-4-fluoro-, 3-[2-[4-(aminoiminomethyl)phenyl]ethoxy]-5-chlorophenyl ester, monoacetate (9CI) (CA INDEX NAME)

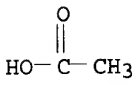
CM 1

CRN 201934-33-0
CMF C21 H17 Cl2 F N2 O4 S

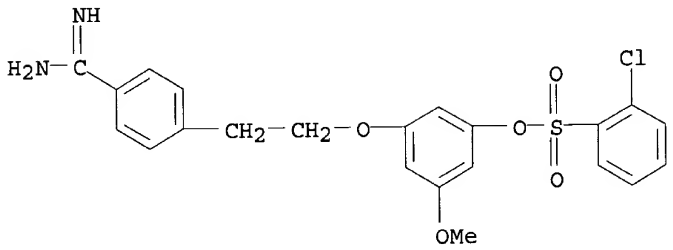


CM 2

CRN 64-19-7
CMF C2 H4 O2

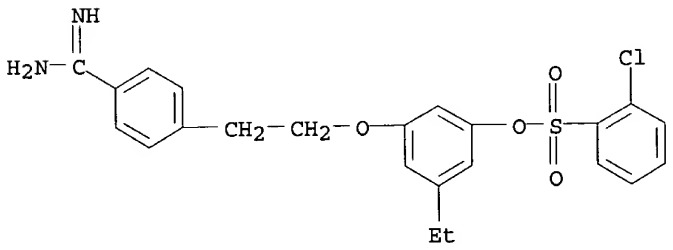


RN 201934-35-2 CAPLUS
CN Benzenesulfonic acid, 2-chloro-, 3-[2-[4-(aminoiminomethyl)phenyl]ethoxy]-5-methoxyphenyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

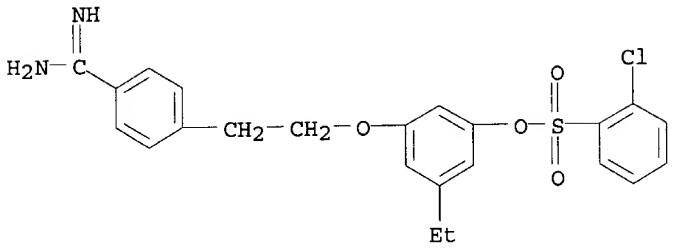
RN 201934-36-3 CAPLUS
CN Benzenesulfonic acid, 2-chloro-, 3-[2-[4-(aminoiminomethyl)phenyl]ethoxy]-5-ethylphenyl ester (9CI) (CA INDEX NAME)



RN 201934-37-4 CAPLUS
CN Benzenesulfonic acid, 2-chloro-, 3-[2-[4-(aminoiminomethyl)phenyl]ethoxy]-5-ethylphenyl ester, monoacetate (9CI) (CA INDEX NAME)

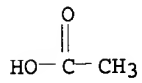
CM 1

CRN 201934-36-3
CMF C23 H23 Cl N2 O4 S

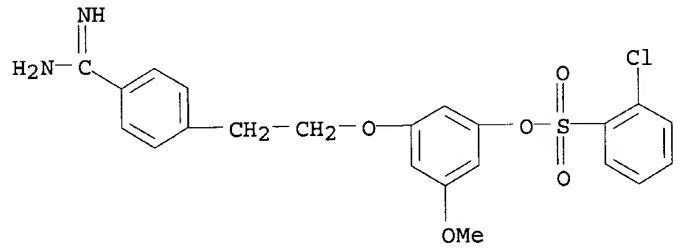


CM 2

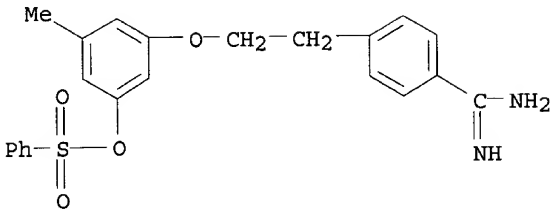
CRN 64-19-7
CMF C2 H4 O2



RN 201934-77-2 CAPLUS
CN Benzenesulfonic acid, 2-chloro-, 3-[2-[4-(aminoiminomethyl)phenyl]ethoxy]-5-methoxyphenyl ester (9CI) (CA INDEX NAME)

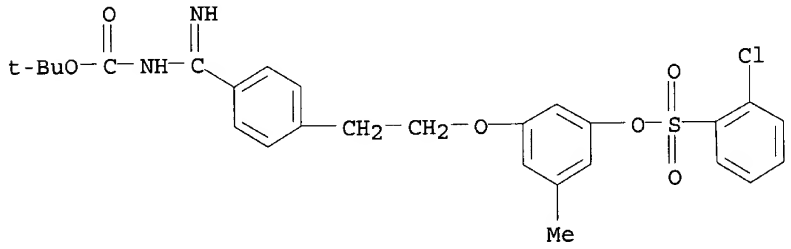


RN 201935-45-7 CAPLUS
CN Benzenecarboximidamide, 4-[2-[3-methyl-5-[(phenylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME)

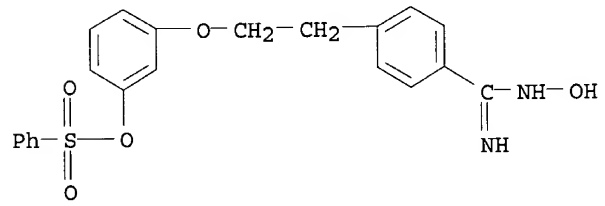


IT **201935-29-7P 201935-31-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of new amidino derivs. as thrombin inhibitors)

RN 201935-29-7 CAPLUS
CN Benzenesulfonic acid, 2-chloro-, 3-[2-[4-[[[(1,1-dimethylethoxy)carbonyl]amino]iminomethyl]phenyl]ethoxy]-5-methylphenyl ester (9CI) (CA INDEX NAME)



RN 201935-31-1 CAPLUS
CN Benzenecarboximidamide, N-hydroxy-4-[2-[3-[(phenylsulfonyl)oxy]phenoxy]ethyl]- (9CI) (CA INDEX NAME)



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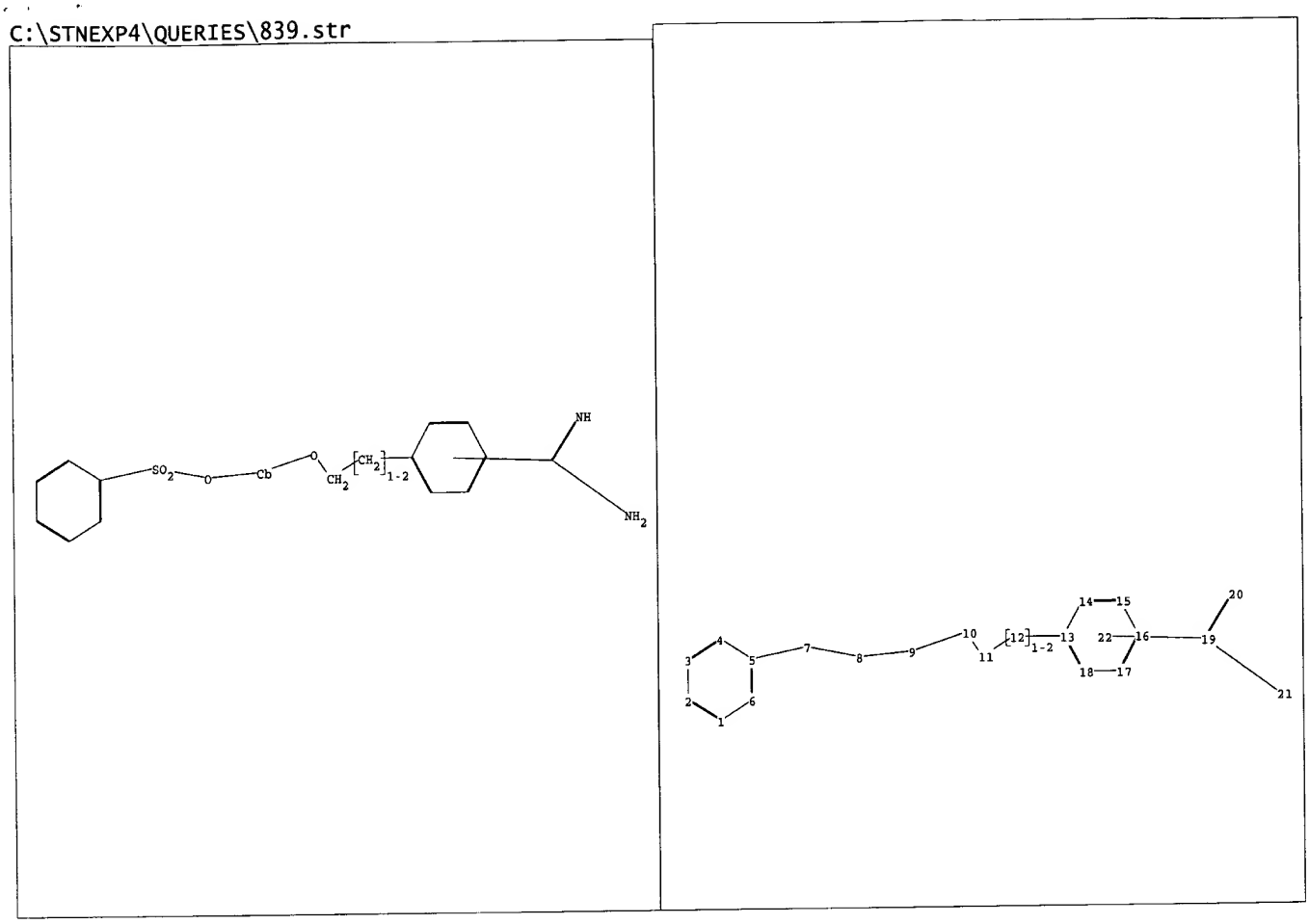

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7 8 9 10 11 12 19 20 21
ring nodes :
1 2 3 4 5 6 13 14 15 16 17 18
chain bonds :
5-7 7-8 8-9 9-10 10-11 11-12 12-13 19-20 19-21
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18
exact/norm bonds :
7-8 19-20 19-21
exact bonds :
5-7 8-9 9-10 10-11 11-12 12-13
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS
20:CLASS 21:CLASS 22:CLASS
Generic attributes :
9:
Saturation : Unsaturated
Number of Carbon Atoms : less than 7
Type of Ring System : Monocyclic

Element Count :
Node 9: Limited
C,C6